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# **33<sup>rd</sup> Asilomar Conference on Mass Spectrometry**

## **IMPACT OF METABOLOMICS IN TRANSLATIONAL AND CLINICAL RESEARCH**

**Friday, September 29 - Tuesday, October 3, 2017**  
**Asilomar Conference Center, Pacific Grove, CA**

### **Organizers**

**Timothy J. Garrett**

*University of Florida and Southeast Center for Integrated Metabolomics*

**Christopher Petucci**

*Sanford Burnham Prebys Medical Discovery Institute*

### **Table of Contents**

|  |    |
|--|----|
| General Information .....                          | 1  |
| Map of Asilomar Conference Grounds .....           | 2  |
| Friday Sessions .....                              | 3  |
| Saturday Sessions .....                            | 4  |
| Friday-Saturday Posters (presented Sat. eve) ..... | 5  |
| Sunday Sessions .....                              | 8  |
| Sunday-Monday Posters (presented Sun. eve) .....   | 9  |
| Monday Sessions .....                              | 11 |
| Participant Directory .....                        | 13 |

### **ASMS Asilomar Committee**

**David Arnott**  
**Genentech**

**Lingjun Li**  
**University of Wisconsin-Madison**

**Benjamin Garcia**  
**University of Pennsylvania**

**Jenny Brodbelt, Board Representative**  
**University of Texas at Austin**

## NOTES

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## GENERAL INFORMATION

### INTERNET ACCESS

There is complimentary wi-fi access in the session room (Chapel), guest rooms and the Social Hall (main building).

To use the wi-fi in Chapel (session room), please follow these instructions:

- Connect to the Asilomar Conference Network
- Passphrase is the word "conference" (lowercase)
- Once connected, open your web browser.
- You should see Asilomar Conf. Grounds login page.
- Scroll to the bottom of the page and use the Username and Password below:

Username: conf8690

Password: conf8690

### MEALS AT ASILOMAR

For attendees lodging at Asilomar you will receive meal tickets for all meals beginning with dinner on Friday and ending with lunch on Tuesday. A vegetarian option is always available upon request at the meal line. *For Tuesday a box lunch has been requested for you, please use your remaining lunch ticket to pick up your box lunch on Tuesday morning, 7:30-9:00 am, outside the Woodlands section of main dining hall. Woodlands is at the end of main dining hall furthest from the ocean.*

For attendees staying offsite you will have (3) lunch tickets and (3) dinner tickets. If for some reason you did not pay the offsite fee, there will be no tickets for you at registration.

For everyone, to-go lunches are available all days during lunch service hour. Simply go to the regular lunch window and request a "To-Go Lunch".

Conference Banquet. There will be an upgraded meal served in a private room off of the main dining hall served with wine (Seascape). Banquet ticket is required. Please look for signs directing you to the special exterior entrance to Seascape. Dessert will be served at the mixer following the closing session.

### EVENING RECEPTIONS

Friday, Saturday, Sunday, and Monday evenings an informal reception is held in Chapel immediately following the evening session. These evening mixers are an opportunity to continue lively discussion and interact with fellow attendees. Saturday and Sunday evenings look for authors attending their posters. There are two groups of posters (Fri-Sat and Sun-Mon).

### SUNDAY AFTERNOON

There is a free afternoon. Attendees are encouraged to join others for outings. Suggest your own activity or sign up to join others. Sign-up sheets in Chapel.

### PRESENTER GUIDELINES

Invited Speakers and Hot Topic Speakers. Please arrive in the Chapel 15-20 minutes prior to the start of the session to set up your device or load your presentation onto the conference computer (PC). Remember to have your own adapters handy to connect to VGA if using your own device.

Poster Presenters. All posters are located in the Chapel. Poster boards will be numbered. There are two groups of posters, please note the posting and removal times listed below.

#### Friday-Saturday Posters

Mount posters by 6 pm Fri. Remove after Sat. mixer.

#### Sunday-Monday Posters

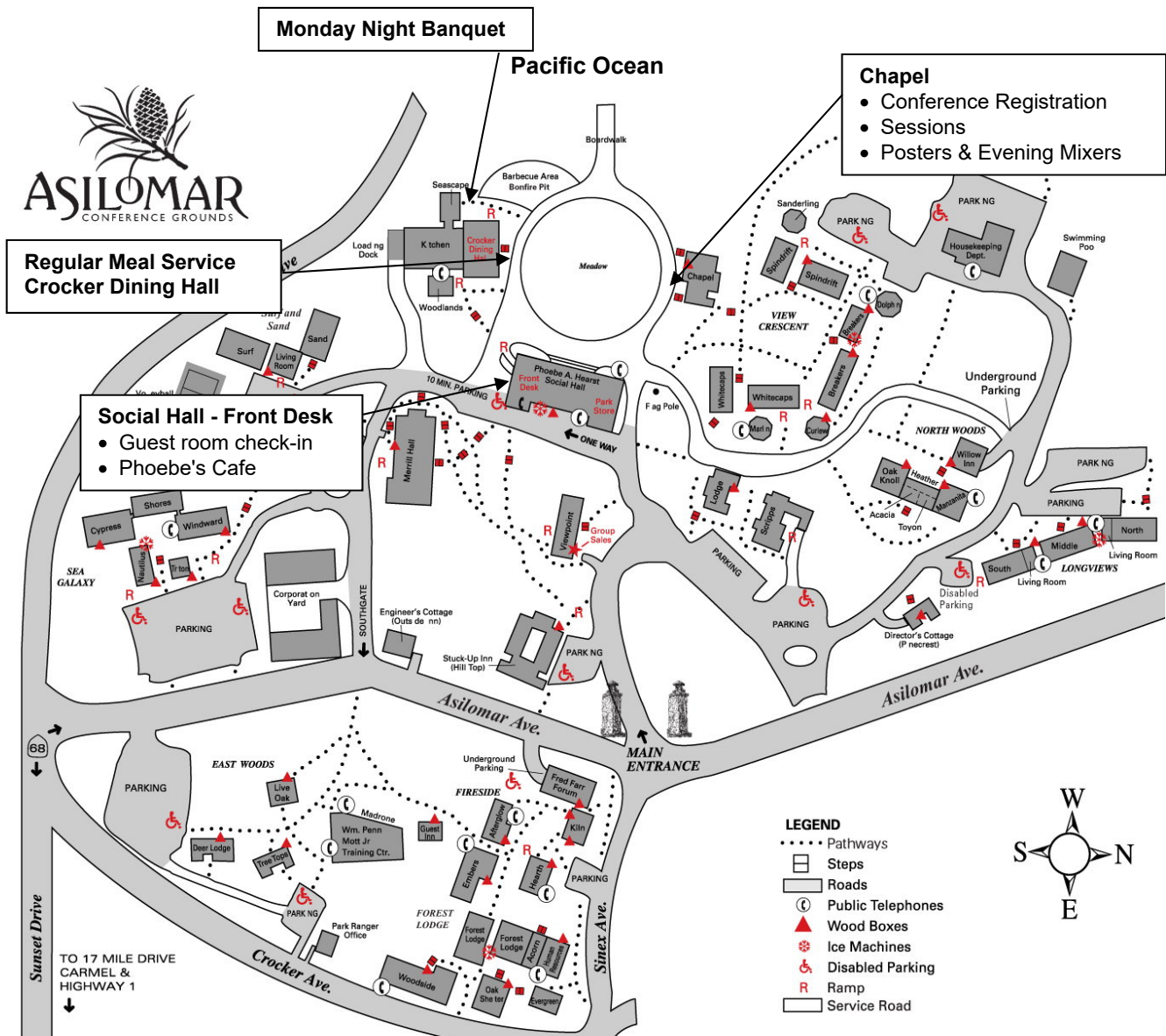
Mount posters by 9 am Sun. Remove after Mon. mixer.

Poster Highlight Talks. Follow instructions you received by email. Please load your 3-min presentation onto the session room laptop (on speaker table) by 6:45 pm the evening of your highlight talk.

### PROGRAM OVERVIEW

|          |  |
|----------|--|
| Friday   | 4:00 - 6:00 pm .....Badge Pickup   |
|          | 6:00 - 7:00 pm .....Asilomar Dinner  |
|          | 7:15 - 8:40 pm .....Session  |
|          | 8:40 - 10:00 pm .....Reception & Posters   |
| Saturday | 7:30 - 9:00 am .....Asilomar Breakfast   |
|          | 9:00 - 10:45 am .....Session   |
|          | 10:45 - 11:05 am .....Coffee Break   |
|          | 11:05 - 11:55 am .....Session  |
|          | 12:00 - 1:00 pm .....Asilomar Lunch  |
|          | 1:15 - 3:00 pm .....Session  |
|          | 3:00 - 3:15 pm .....Group Photo  |
|          | 3:15 - 6:00 pm .....Free Time  |
|          | 6:00 - 7:00 pm .....Asilomar Dinner  |
|          | 7:15 - 7:45 pm .....Session  |
|          | 7:45 - 10:00 pm .....Reception & Posters   |
| Sunday   | 7:30 - 9:00 am .....Asilomar Breakfast   |
|          | 9:00 - 10:10 am .....Session, part 1   |
|          | 10:10 - 10:30 am .....Coffee Break   |
|          | 10:30 - 11:40 am .....Session, part 2  |
|          | 12:00 - 1:00 pm .....Asilomar Lunch  |
|          | 1:00 - 6:00 pm .....Free Afternoon   |
|          | 6:00 - 7:00 pm .....Asilomar Dinner  |
|          | 7:15 - 7:45 pm .....Session  |
|          | 7:45 - 10:00 pm .....Reception & Posters   |
| Monday   | 7:30 - 9:00 am .....Asilomar Breakfast   |
|          | 9:00 - 10:10 am .....Session   |
|          | 10:10 - 10:30 am .....Coffee Break   |
|          | 10:30 am - 12 pm .....Session  |
|          | 12:00 - 1:00 pm .....Asilomar Lunch  |
|          | 1:15 - 3:00 pm .....Session  |
|          | 3:00 - 6:00 pm .....Free Time  |
|          | 6:00 - 7:15 pm .....Banquet (Seascape)   |
|          | 7:30 - 8:30 pm .....Session  |
|          | 8:30 - 10:00 pm .....Dessert & Posters   |
| Tuesday  | 7:30 - 9:00 am .....Asilomar Breakfast   |
|          | 7:30 - 9:00 am .....Box lunch pick-up<br>inside Crocker Dining<br>Hall (Asilomar guests<br>only) |

## ASILOMAR GROUNDS MAP



## MONTEREY BAY AREA ATTRACTIONS

Sunday afternoon is scheduled free time. You are encouraged to relax on your own or with your fellow attendees. Look for sign-ups in the session room for those interested in group activities. Do you have a car and wish to visit the aquarium? Do you want to rent bikes with others and tour around the area? How about kayaking around Monterey Bay admiring sea otters and the renowned kelp forest as you paddle? Do you want to rent some clubs and play golf? **Be an instigator and list your activity on a sign-up sheet for others to join you.**

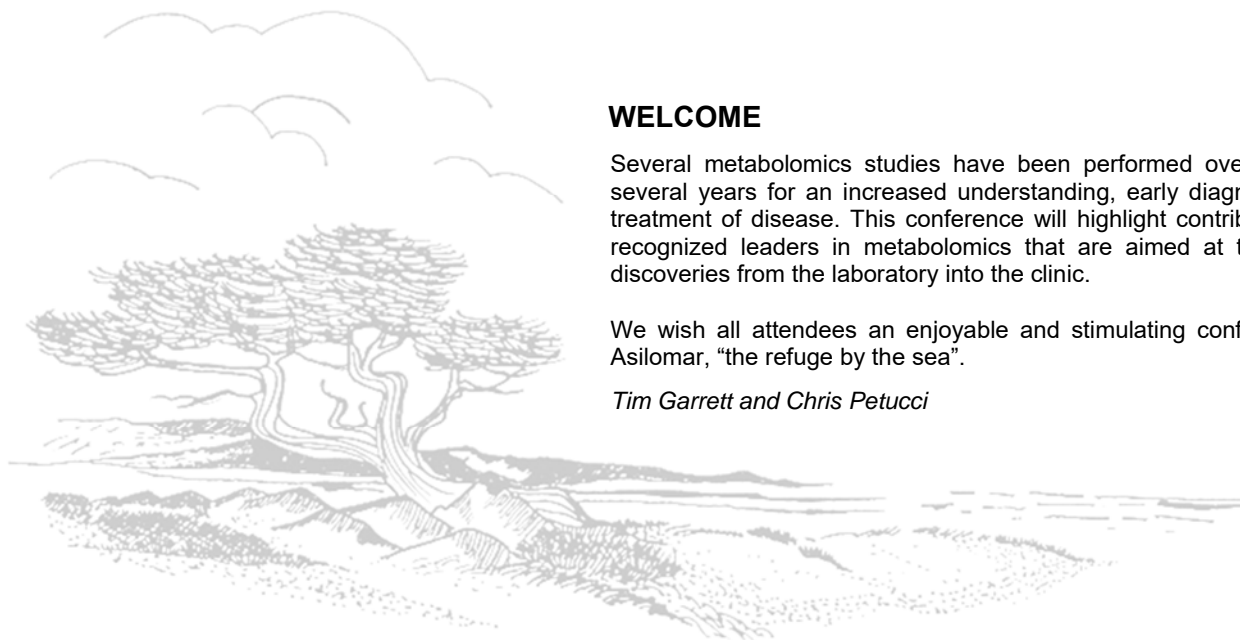
### Some Ideas...

Accessible by foot, bus, bike or car:

- In Monterey - Monterey Bay Aquarium, Fisherman's Wharf, Cannery Row, kayaking on the bay.
- Pebble Beach attractions include the 17-Mile Drive which is accessible free-of-charge on foot or bike or enter by car for a fee.

Accessible by car:

- Carmel Valley is home to many wineries, farms, ranches and the historic Carmel Mission. Hiking in Big Sur or Point Lobos.



## WELCOME

Several metabolomics studies have been performed over the last several years for an increased understanding, early diagnosis, and treatment of disease. This conference will highlight contributions by recognized leaders in metabolomics that are aimed at translating discoveries from the laboratory into the clinic.

We wish all attendees an enjoyable and stimulating conference at Asilomar, "the refuge by the sea".

*Tim Garrett and Chris Petucci*

## FRIDAY, SEPTEMBER 29, 2017

4:00 - 6:00 pm: Registration in *Chapel*  
Materials will also be available for pick-up during the sessions.

6:00 - 7:00 pm: Asilomar Dinner, *Crocker Dining Hall*  
*Meal ticket required.*

7:15 - 8:40 pm: **WELCOME + APPLICATIONS OF TRANSLATIONAL AND GLOBAL METABOLOMICS**, *Chapel*  
Session Chair: *Tim Garrett, University of Florida*  
*There is a five-minute gap after each talk for Q&A.*

- |                |   |
|----------------|---|
| 7:15 - 7:25 pm | Opening Remarks; Tim Garrett and Chris Petucci  |
| 7:25 - 7:55 pm | <b>LC-MS/MS-based Approach Helps Identify a New Mechanism for Multiple Sclerosis in a Mouse Model</b> ; Sunia Trauger, <i>Harvard University</i>                              |
| 8:00 - 8:30 pm | <b>Early Detection of Cystic Fibrosis Acute Pulmonary Exacerbations by Exhaled Breath Condensate Metabolomics</b> ; Facundo Fernandez, <i>Georgia Institute of Technology</i> |
| 8:35 - 8:45 pm | About the Asilomar Conference and Welcome to the Reception, Ben Garcia, <i>ASMS Asilomar Committee</i>  |

8:45 - 10:00 pm: **RECEPTION AND FRIDAY-SATURDAY POSTERS**, *Chapel*

Special thanks to this evening's reception sponsor  
**SCIEX**

*Friday-Saturday Posters on display. See Friday-Saturday Poster Group listing on pages 5-6.*

## SATURDAY, SEPTEMBER 30, 2017

7:30 - 9:00 am: Asilomar Breakfast (onsite lodgers only), *Crocker Dining Hall*  
*If you are staying offsite, you may purchase a breakfast meal ticket at the Asilomar Front Desk.*

9:00 - 10:45 am: **CLINICAL APPLICATIONS OF GLOBAL METABOLOMICS**, *Chapel*  
Session Chair: Abraham Badu-Tawiah, *The Ohio State University*

*There is a five-minute gap after each talk for Q&A.*

- 9:00 - 9:30 am     **Tracking Electrons with Metabolomics Reveals Therapeutic Vulnerabilities in Cancer**; Gary Patti, *Washington University at St. Louis*
- 9:35 - 10:05 am   **Using Metabolomics to Predict Treatment Response in a Pediatric Asthma Population**; Nichole Reisdorph, *University of Colorado*
- 10:10 - 10:40 am   **Time for Metabolomics: Translational Studies in Chronobiology and Cancer**; Aalim Weljie, *University of Pennsylvania*

10:45 - 11:05 am: **COFFEE BREAK**

11:05 - 11:55 am: **HOT TOPIC TALKS selected from submitted abstracts**, *Chapel*  
Session Chair: Chris Petucci, *Sanford Burnham Prebys Medical Discovery Institute*

*There is a five-minute gap after each talk for Q&A.*

- 11:05 - 11:25 am   **Dynamic Changes in the Microbiome and Fecal Metabolome in Patients Undergoing Hematopoietic Stem Cell Transplantation**; Justin Cross, *Memorial Sloan Kettering Cancer Center*
- 11:30- 11:50 am    **3D Volume Cartography of Diseased Human Lungs**; Alexey Melnik, *University of California, San Diego*

12:00 - 1:00 pm: Asilomar Lunch, *Crocker Dining Hall*  
*Meal ticket required.*

1:15 - 3:00 pm: **CLINICAL APPLICATIONS OF TARGETED METABOLOMICS**, *Chapel*  
Session Chair: Michelle Clasquin, *Pfizer*

*There is a five-minute gap after each talk for Q&A.*

- 1:15 - 1:45 pm     **Metabolomics in Solid Organ Transplantation: The Right Tool for "Right Now"**; John Seal, *Ochsner Mutli-Organ Transplant Institute*
- 1:50 - 2:20 pm     **Opportunities and Challenges in Translating Metabolomics Findings into Cancer Related Diagnostic Tests**; Dan Raftery, *University of Washington*
- 2:25 - 2:55 pm     **Metabolomic Methods to Identify Early Metabolic Indicators of Subclinical Disease in Human Cohorts**; Clary Clish, *Broad Institute of MIT and Harvard*

3:00 - 3:15 pm: **GROUP PHOTO**

3:15 - 6:00 pm: **FREE TIME**

6:00 - 7:00 pm: Asilomar Dinner, *Crocker Dining Hall*  
*Meal ticket required.*

## SATURDAY, SEPTEMBER 30, 2017, *continued*

7:15 – 7:45 pm: **POSTER HIGHLIGHT TALKS**, Chapel

Session Chair: Chris Petucci, Sanford Burnham Prebys Medical Discovery Institute

*Brief three minute presentations intended to highlight some of the posters from the Friday-Saturday Poster Group.*

- |                |  |
|----------------|--|
| 7:15 - 7:18 pm | <b>Using Desorption Electrospray Ionization to Diagnose Primary and Metastatic Melanoma Staging;</b> <u>Alena Bensussan</u> , University of Texas Austin, Austin, TX   |
| 7:19 - 7:22 pm | <b>Urinary Metabolome of Inflammatory Bowel Diseases: Elucidating the Impact of Exclusive Enteral Nutrition Therapy as an Alternative to Corticosteroid Treatment;</b> <u>Mai Yamamoto</u> , Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON |
| 7:23 - 7:26 pm | <b>Explore metabolic flux in Rothia mucilaginosa using U-13C glucose tracer;</b> <u>Bei Gao</u> , UC Davis, Davis  |
| 7:27 - 7:30 pm | <b>Dysregulation of phosphatidylcholine and cholesterol ester metabolisms at prodromal stage of Late Onset Alzheimer's Disease;</b> <u>Min Kim</u> , King's College London, London, United Kingdom   |
| 7:31 - 7:34 pm | <b>Formation of Steroid Multimer Adducts Implications on Isomer Discrimination with Ion Mobility-Mass Spectrometry;</b> <u>Alana Rister</u> , University of Nebraska, Lincoln, NE  |
| 7:40 - 7:45 pm | <b>Welcome to this evening's reception sponsored by SCIEX</b>  |

7:45 - 10:00 pm: **FRIDAY-SATURDAY POSTERS AND INFORMAL MIXER**, Chapel

Special thanks to this evening's reception sponsor  
**SCIEX**

The Friday-Saturday Posters will be displayed from 6:00 pm, Friday – 10:00 pm, Saturday night.  
Posters will be presented (attended by author) during the Saturday evening reception.

### Poster Number

- |            |  |
|------------|--|
| Fri/Sat 1  | <b>Quantitative Imaging of Brain Metabolites using DESI MSI with Stable Isotope Labels;</b> <u>Bindesh Shrestha</u> , Waters Corp., Beverly, MA  |
| Fri/Sat 2  | <b>Using Desorption Electrospray Ionization to Diagnose Primary and Metastatic Melanoma Staging;</b> <u>Alena Bensussan</u> , University of Texas Austin, Austin, TX   |
| Fri/Sat 3  | <b>Tools to Understand the Gut Microbiome: A Refined LC-MS/MS Method to Profile Bacteria-derived Bile Acids;</b> <u>Mark Sartain</u> , Agilent Technologies, Santa Clara, CA   |
| Fri/Sat 4  | <b>UHPLC-HRMS detection of U13C labeled glucose for metabolic analysis of exercise impact on heart and skeletal muscle;</b> <u>Michelle Reid</u> , University of Florida, Gainesville, FL  |
| Fri/Sat 5  | <b>Urinary Metabolome of Inflammatory Bowel Diseases: Elucidating the Impact of Exclusive Enteral Nutrition Therapy as an Alternative to Corticosteroid Treatment;</b> <u>Mai Yamamoto</u> , Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON |
| Fri/Sat 6  | <b>Metabolomics Strategies on Cytochrome P450 Reaction Phenotyping Assays;</b> <u>Xuejun Peng</u> , Bruker Daltonics, Billerica, MA  |
| Fri/Sat 7  | <b>Metabolomics reveals differences in metabolic pathways predictive of recovery of renal function following liver transplantation;</b> <u>Stephen Barnes</u> , University of Alabama at Birmingham, Birmingham, AL  |
| Fri/Sat 8  | <b>Assessment of Ketogenic Diets as Adjuvant Treatment of Neuroblastoma in a Mouse Model by Metabolomic Profiling;</b> <u>David Licha</u> , University of Salzburg, Department of Molecular Biology, Division of Chemistry and Bioanalytics, Salzburg, Austria               |
| Fri/Sat 9  | <b>Spatial Mapping of Glycosphingolipids using MALDI Mass Spectrometry Imaging: Insights for Gene Therapy in a Murine Model of GM1 Gangliosidosis;</b> <u>Scott A. Shaffer</u> , University of Massachusetts Medical School, Worcester, MA                                   |
| Fri/Sat 10 | <b>Explore metabolic flux in Rothia mucilaginosa using U-13C glucose tracer;</b> <u>Bei Gao</u> , UC Davis, Davis  |
| Fri/Sat 11 | <b>Monitoring the dynamics of 13C Palmitate absorption and metabolism in the plasma and tissues of Zucker rats;</b> <u>Mahmoud ElAzzouny</u> , Agilent Technologies, Santa Clara, CA   |

**SATURDAY, SEPTEMBER 30, 2017, *continued***

- Fri/Sat 12    **Untargeted in vitro Metabolomics: Dose-Response Analysis and Comparisons to Transcriptomic Analysis;** David Crizer, *National Toxicology Program/NIEHS/NIH, Research Triangle Park, NC*
- Fri/Sat 13    **Dysregulation of phosphatidylcholine and cholesterol ester metabolisms at prodromal stage of Late Onset Alzheimer's Disease;** Min Kim, *King's College London, London, United Kingdom*
- Fri/Sat 14    **Metabolomic Biomarkers for Human Plasma Quality by UHPLC-HRMS;** Casey Chamberlain, *University of Florida, Gainesville, FL*
- Fri/Sat 15    **Formation of Steroid Multimer Adducts Implications on Isomer Discrimination with Ion Mobility-Mass Spectrometry;** Alana Rister, *University of Nebraska, Lincoln, NE*
- Fri/Sat 16    **Examples of Metabolite Biomarker Assays in Drug Development by LC-MS-MS;** Michael Sullivan, *Worldwide Clinical Trials, Austin, TX*
- Fri/Sat 17    **Pan-Cancer Profiling of Cell Line Lysates by Untargeted Metabolomics;** Jennifer Dennison, *University of Texas MD Anderson Cancer Center, Houston*
- Fri/Sat 18    **Development of New NIST Metabolomics Reference Materials and Data;** Christina Jones, *National Institute of Standards and Technology, Gaithersburg, MD*

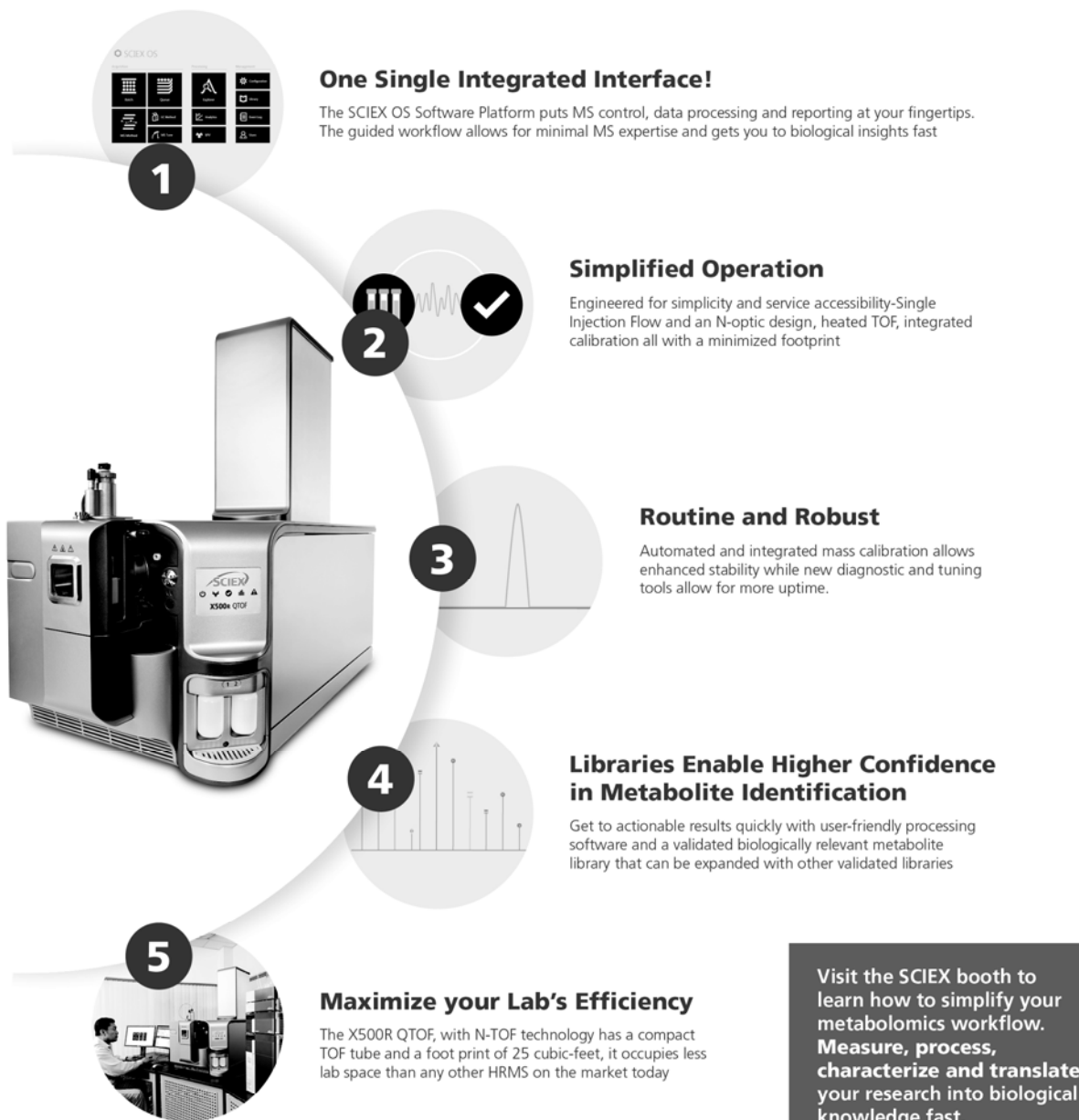


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02/2017 RUO-MKT-07-5081-A

## SUNDAY, OCTOBER 1, 2017

7:30 - 9:00 am: Asilomar Breakfast (onsite lodgers only), *Crocker Dining Hall*  
*If you are staying offsite, you may purchase a breakfast meal ticket at the Asilomar Front Desk.*

### SUNDAY-MONDAY POSTERS

*Sunday-Monday Posters on display this morning through Monday night. See complete listing on pages 12 - 13.*

9:00 am - 11:40 am: **CLINICAL APPLICATIONS OF NEW TECHNOLOGY: AMBIENT DESORPTION IONIZATION/MS IMAGING/ION MOBILITY**, *Chapel*

Session Chair: Facundo Fernandez, *Georgia Institute of Technology*

*There is a five-minute gap after the each talk for Q&A.*

9:00 - 9:30 am     **Ionic Probes for Mass Spectrometry Signal Amplification and Application in Paper-based On-Demand Diagnostics**; Abraham Badu-Tawiah, *The Ohio State University*

9:35 - 10:05 am     **Precision surgery: Translational Applications of Ambient Mass Spectrometry in the Operating Room**; James Kinross, *Imperial College*

10:10 - 10:30 am: **COFFEE BREAK**

10:30 - 11:00 am     **Sub-Minute Small Molecule Screenings of Biofluid and Environmental Samples Using Ion Mobility Spectrometry Coupled with Mass Spectrometry**; Erin Baker, *PNNL*

11:05 - 11:35 am     **Rapid Response Precision Microbiome - Multi-omics Analysis at Clinical Relevant Time Scales**; Pieter Dorrestein, *University of California, San Diego*

12:00 - 1:00 pm: Asilomar Lunch, *Crocker Dining Hall*  
*Meal ticket required.*

1:00 - 6:00 pm: Free Afternoon

6:00 - 7:00 pm: Asilomar Dinner, *Crocker Dining Hall*  
*Meal ticket required.*

7:15 - 7:45 pm: **POSTER HIGHLIGHT TALKS**, *Chapel*

Session Chair: Tim Garrett, *University of Florida*

*Brief three minute presentations intended to highlight some of the posters from the Sunday-Monday Poster Group.*

7:15 - 7:18 pm     **Comparison and Optimization of SWATH to Information-Dependent Acquisition for Small Molecule Analysis**; Jeffrey Whitman, *University of California, San Francisco, San Francisco, CA*

7:19 - 7:22 pm     **Molecular Discrimination of Follicular Thyroid Adenomas and Carcinomas using Desorption Electrospray Ionization Mass Spectrometry**; Rachel DeHoog, *University of Texas Austin, Austin, TX*

7:23 - 7:26 pm     **Mass Spectrometric Investigation of the Human Gut Microbiota's Response to Infection as a Source for Novel Antibiotics**; Caitlin Keller, *University of Wisconsin, Madison, WI*

7:27 - 7:30 pm     **Polyphenols Regulate Diet-Gut Microbiota Interactions in a Mouse Obesity Model**; Johana Revel, *OSU, Department of Chemistry, Corvallis, OR*

7:31 - 7:34 pm     **A Structural Examination and Collision Cross Section Database for Over 500 Metabolites and Xenobiotics Using Drift Tube Ion Mobility Spectrometry**; Xueyun Zheng, *Pacific Northwest National Laboratory, Richland, WA*

7:40 - 7:45 pm     **Welcome to this evening's reception sponsored by Waters Corporation**, Bindesh Shrestha,

## SUNDAY, OCTOBER 1, 2017, *continued*

7:45 - 10:00 pm: **SUNDAY-MONDAY POSTERS AND INFORMAL MIXER**, *Chapel*

Special thanks to this evening's reception sponsor  
**Waters Corporation**

The Sunday-Monday Posters will be displayed from 9:00 am, Sunday – 10:00 pm, Monday night.  
Posters will be presented (attended by author) during the Saturday evening reception.

### *Poster Number*

- |            |   |
|------------|---|
| Sun/Mon 1  | <b>Metabolic Reprogramming and Redox Adaptation in Sorafenib-Resistant Leukemia Cells: Detected by Untargeted Metabolomics and Stable Isotope Tracing Analysis;</b> <u>Yumin Hu</u> , <i>Sun Yat-sen University Cancer Center, Guangzhou, China</i> |
| Sun/Mon 2  | <b>Comparison and Optimization of SWATH to Information-Dependent Acquisition for Small Molecule Analysis;</b> <u>Jeffrey Whitman</u> , <i>University of California, San Francisco, San Francisco, CA</i>  |
| Sun/Mon 3  | <b>Longitudinal Metabolic Profiling During Health and Disease in Prediabetic Individuals;</b> <u>Kevin Contrepois</u> , <i>Stanford University, Stanford</i>  |
| Sun/Mon 4  | <b>ADAP-3D: Peak Detection Method for LC/ and GC/MS Profile Metabolomics Data which Considers the Data's Three-Dimensions to Reduce False Positives;</b> <u>Xiuxia Du</u> , <i>University of North Carolina at Charlotte, Charlotte, NC</i>         |
| Sun/Mon 5  | <b>Molecular Discrimination of Follicular Thyroid Adenomas and Carcinomas using Desorption Electrospray Ionization Mass Spectrometry;</b> <u>Rachel DeHoog</u> , <i>University of Texas Austin, Austin, TX</i>                                      |
| Sun/Mon 6  | <b>Creation of a Bile Acids Spectral Library to Investigate the Gut Microbiome with Elements for Metabolomics;</b> <u>Jacob Lippincott</u> , <i>Proteome Software, Portland, OR</i>   |
| Sun/Mon 7  | <b>Mass Spectrometric Investigation of the Human Gut Microbiota's Response to Infection as a Source for Novel Antibiotics;</b> <u>Caitlin Keller</u> , <i>University of Wisconsin, Madison, WI</i>  |
| Sun/Mon 8  | <b>Skyline for Targeted Metabolomics;</b> <u>Brian Pratt</u> , <i>University of Washington, Seattle, WA</i>   |
| Sun/Mon 9  | <b>Polyphenols Regulate Diet–Gut Microbiota Interactions in a Mouse Obesity Model;</b> <u>Johana Revel</u> , <i>OSU, Department of Chemistry, Corvallis, OR</i>   |
| Sun/Mon 10 | <b>Untargeted Metabolomic Profiling of the Epitranscriptome: Discovery of New Modified Nucleobases in RNA for Clinical Diagnostics;</b> <u>Megan Showalter</u> , <i>UC Davis, Davis, CA</i>   |
| Sun/Mon 11 | <b>Evidence of Multiple Pools of Glucose-6-phosphate from Combined Metabolomics and Fluxomic Studies in Perfused Muscle;</b> <u>Natalie Daurio</u> , <i>Merck, Kenilworth, NJ</i>   |
| Sun/Mon 12 | <b>Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a Tool for Assigning Isotopologues and Metabolites in Fourier Transform Mass Spectra;</b> <u>Hunter Moseley</u> , <i>University of Kentucky, Lexington, KY</i>                      |
| Sun/Mon 13 | <b>Multi-omics Profiling of LKB1 Mutant NSCLCs Cells to Characterize Deregulated Pathways Contributing to Tumorigenesis;</b> <u>Bernice Agana</u> , <i>The Ohio State University, Columbus, OH</i>  |
| Sun/Mon 14 | <b>A Structural Examination and Collision Cross Section Database for Over 500 Metabolites and Xenobiotics Using Drift Tube Ion Mobility Spectrometry;</b> <u>Xueyun Zheng</u> , <i>Pacific Northwest National Laboratory, Richland, WA</i>          |
| Sun/Mon 15 | <b>Biomarker Driven Approach to Determine Unfavorable Outcomes in Diabetic Pregnant Women by Automated MALDI Magnetic Resonance Mass Spectrometry and NMR;</b> <u>Franklin E. Leach III</u> , <i>University of Georgia, Athens, GA</i>              |
| Sun/Mon 16 | <b>Stable Isotope Labeled Pyruvate Tolerance Test;</b> <u>Xiaoyang Su</u> , <i>Division of Endocrinology, Departments of Medicine, Robert Wood Johnson Medical School, Rutgers University, New Brunswick, NJ</i>                                    |
| Sun/Mon 17 | <b>Toward Establishing Standardized Protocol for Untargeted LC–MS-based Lipidomics Analysis for Use in Clinical Laboratories;</b> <u>Tomas Cajka</u> , <i>West Coast Metabolomics Center, University of California Davis, Davis, CA</i>             |

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# THERE ARE THREE DIMENSIONS OF RESOLUTION.

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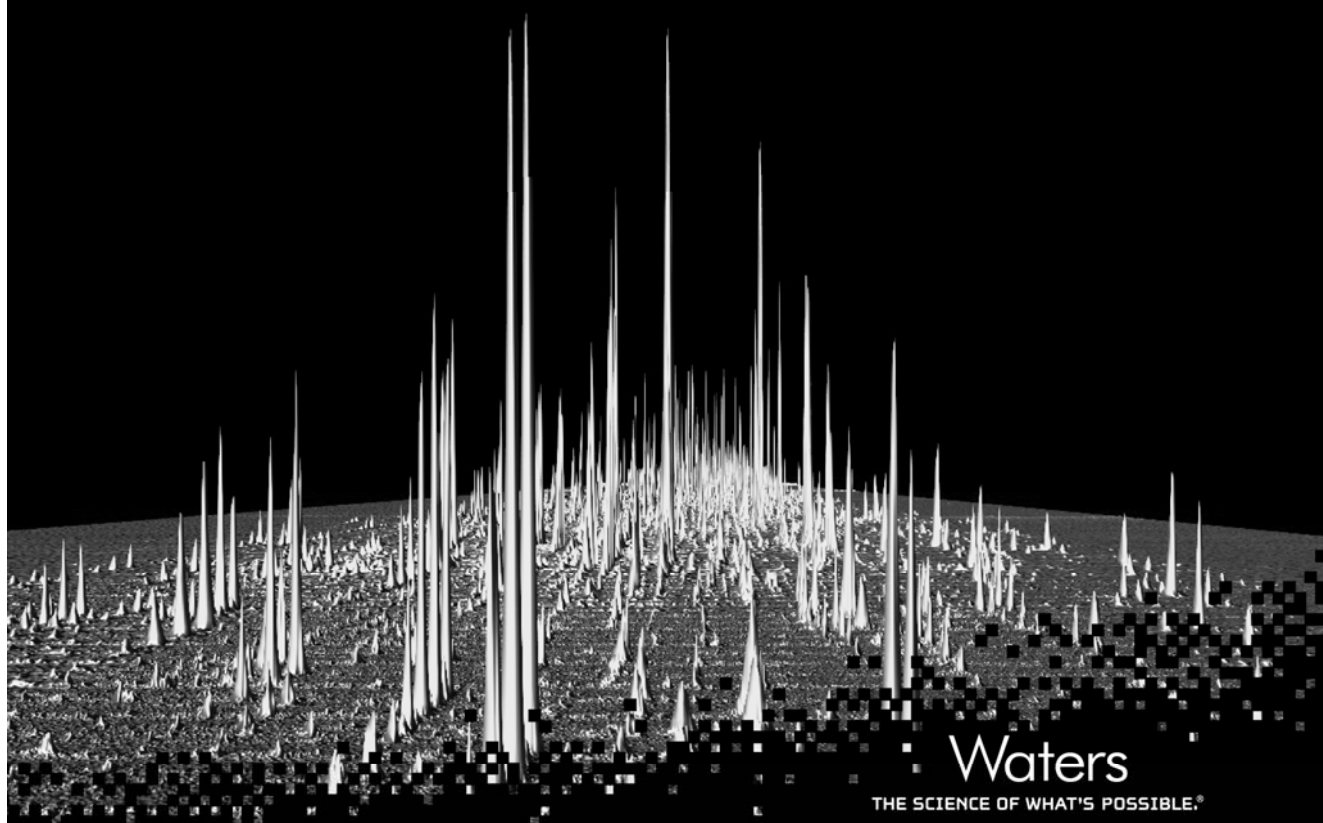
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## MONDAY, OCTOBER 2, 2017

7:30 - 9:00 am: Asilomar Breakfast (onsite lodgers only), *Crocker Dining Hall*  
*If you are staying offsite, you may purchase a breakfast meal ticket at the Asilomar Front Desk.*

9:00 am - 10:10 am: **TRANSLATIONAL AND CLINICAL APPLICATIONS OF METABOLIC FLUX  
BY MASS SPECTROMETRY**, *Chapel*

Session Chair: Dan Raftery, *University of Washington*

*There is a five-minute gap after each talk for Q&A.*

- 9:00 - 9:30 am     **Stable Isotope <sup>18</sup>O-assisted Dynamic Metabolomics: Experimental and Clinical Applications;**  
Petrás Dzeja, *Mayo Clinic*
- 9:35 - 10:05 am   **Drug Discovery Guided by MIMOSA Mass Isotopomer Flux Analysis;** Richard Kibbey, *Yale School  
of Medicine*

10:10 – 10:30 am: **COFFEE BREAK**

10:30 am - 12:00 pm: **METABOLOMICS APPLICATIONS IN THE PHARMACEUTICAL INDUSTRY**, *Chapel*

Session Chair: Erin Baker, *PNNL*

*There is a five-minute gap after each talk for Q&A.*

- 10:30 - 10:55 am   **Metabolomics Based Approach to Drug Discovery and Development;** Alla Kloss, *Genzyme*
- 11:00 - 11:25 am   **Metabolomics Applications in the Discovery of Safety Biomarkers in Preclinical Development;**  
Yutai Li, *Merck*
- 11:30 - 11:55 am   **Understanding Disease through Unlabeled and Isotope Tracer-based Metabolomics and  
Lipidomics;** Michelle Clasquin, *Pfizer*

12:00 - 1:00 pm: Asilomar Lunch (all attendees), *Crocker Dining Hall*  
*Meal ticket required.*

1:15 - 3:00 pm: **NIH REGIONAL COMPREHENSIVE METABOLOMICS RESEARCH CORES: INNOVATIONS AND  
CLINICAL APPLICATIONS**, *Chapel*

Session Chair: Nichole Reisdorph, *University of Colorado*

*There is a five-minute gap after each talk for Q&A.*

- 1:15 - 1:45 pm     **Mass Spectrometric Innovations for Translational and Clinical Research;** Rick Yost, *University of  
Florida*
- 1:50 - 2:20 pm     **Challenges of Metabolic Reprogramming Elucidation in Cancers Directly from Human Subjects  
via SIRM-mass Spectrometry;** Rick Higashi, *University of Kentucky*
- 2:25 – 2:55 pm     **Standardizing Non-targeted Metabolomics for use in Clinical Research;** Oliver Fiehn, *University of  
California, Davis*

3:00 - 6:00 pm: **FREE TIME**

## MONDAY, OCTOBER 2, 2017, *continued*

6:00 - 7:15 pm: **BANQUET DINNER**

*Look for signs guiding you to Seascape exterior entrance located toward the ocean from main dining hall stairs.  
Bring your ASMS banquet ticket! If you need a ticket, please see Brent in rear of Chapel.*

7:30 - 8:30 pm: **KEYNOTE TALK + CLOSING SESSION**, Chapel  
Session Chair: Chris Petucci, *Sanford Burnham Prebys Medical Discovery Institute*

7:30 - 8:15 pm     **Translating Metabolomics into Activity using the Fox Force Five**; Gary Siuzdak, *The Scripps Research Institute*

8:20 - 8:25 pm     Closing Remarks from Tim Garrett and Chris Petucci

8:30 - 10:00 pm: **DESSERT AND SUNDAY-MONDAY POSTERS**, Chapel

*Sunday-Monday Posters on display. See Sunday-Monday Poster Group listing on page 9.*

## TUESDAY, OCTOBER 3, 2017

7:30 - 9:00 am: Asilomar Breakfast, *Crocker Dining Hall*

7:30 - 9:00 am: Box Lunch Pick-up for Asilomar Guests, *Social Hall Deck*

*Departures at Leisure*